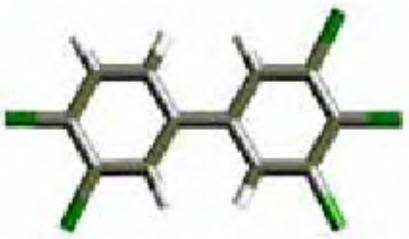
In this issue

Toxicity analysis of PCB

The pollution caused by polychlorinated biphenyls (PCB) has attracted a widespread concern. They are also environmental contaminants due to their capacity of persistence and lipophilicity, biological accumulation into the food chain and concentration in fatty tissues. Defining appropriate descriptors to model reactivity of these molecular systems is the key parameter for development of QSAR and structure-based toxicity prediction. Chemical reactivity descriptors based on DFT are useful in analysing the toxicities



and in identifying the reactive sites. Global reactivity profiles and local selectivity profiles of 33′44′5-pentachloro biphenyl are analysed by Parthasarathi *et al.* (**page 535**) to gain deeper insights into the toxic nature of this compound. Both global and local electrophilicity have been found to be adequate in explaining the overall toxicity and the most probable site of reactivity. Interaction between PCB and nucleic acid bases/selected base pairs and charge transfer involved in the formation of adducts are determined. The results revealed the electron accepting nature of PCBs in their interaction with biomolecules.

Water resources in India

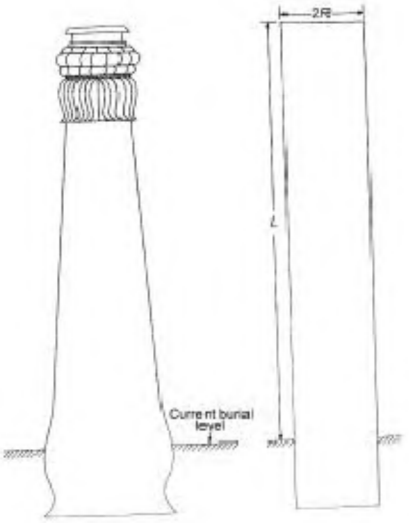
While issues related to water attract considerable attention in all spheres of life in India, very little quantitative information is available on the water budget of the country. Shankar *et al.* (**page 543**) assemble a framework for quantifying India's water resources, and apply it to the Mandovi river in Goa. The framework scales well and is extensible to the entire subcontinent, making it a valuable tool for evaluating the water budget of the river basins of India.

Sniffing a single molecule using biometallic nanoparticles

Surface-enhanced Raman scattering (SERS) spectroscopy is becoming a useful technique to probe nanoparticle–molecule binding through enhanced vibrational band structure. Although the SERS effect on roughened silver electrode was established by Fleischmann and group in 1974, the role of nanostructures and their specific configurations have been realized only recently. An enhancement factor of 14–15 orders of magnitude has been achieved enabling detection of single molecules. At present, it is believed that both a long-range electromagnetic (EM) effect and a short-range chemical effect (modification of molecular dipole due to charge transfer) are operative to describe the surface optical enhancement. In an effort to realize the relative importance of these two mechanisms, Mandal *et al.* (**page 556**) have put forward the SERS enhancement of crystal violet molecules adsorbed on size specific 'Au_{core}–Ag_{shell}' nanocrystals and show that single molecule SERS occurs at the junction of two aggregated particles.

Corrosion resistance of the Delhi iron pillar

The relatively low humidity atmospheric condition of New Delhi has been proposed as one of the main causes for the Delhi iron pillar's excellent atmospheric corrosion resistance. In order to verify this hypothesis, Halder *et al.* (**page 559**) explore the role of atmospheric conditions at Delhi on the wetting of the pillar surface utilizing a non-steady state heat transfer model. Based on available weather conditions of New Delhi, the total wetting time of the pillar, due to moisture condensation and to rainfall, has been computed for one complete year. The wetting time has been used to conservatively estimate the anticipated rust thickness on the pillar. As this is much higher than the actual rust thickness on the pillar, it has been emphasized that the pillar owes its excellent corrosion resistance to the formation of a protective passive film. The environment plays only a contributory role.



Cry2A protein analysis

Shantanu Kumar *et al.* (**page 566**) report susceptibility of the cotton bollworm, *Helicoverpa armigera* to Cry2Aa protein encoded by the gene cloned from an indigenous isolate of *Bacillus thuringiensis* (*Bt*). Commercial cultivars of transgenic *Bt*-cotton in India express Cry1Ac. Continuous exposure of insect pests to a single kind of *Bt* toxin can lead to a rapid development of resistance in insects. Scientists of the CSIRO, Australia have documented that the Cry1Ac-resistant *H. armigera* was not cross-resistant to Cry2Aa. Cloning of indigenous *Bt* genes and identification of structurally different Cry proteins effective against target pests will reduce dependency on foreign companies and will provide basic materials to develop better versions of indigenous transgenic crop plants.